DISPERSED-FLUORESCENCE SPECTROSCOPY OF JET-COOLED CALCIUM ETHOXIDE RADICAL ($CaOC_2H_5$)

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Metal-containing free radicals are important intermediates in metal-surface reactions and in the interaction between metals and organic molecules. In the present work, dispersed fluorescence (DF) spectra of the calcium ethoxide radical ($CaOC_2H_5$) have been obtained by pumping the $\tilde{A}^2\mathrm{A}' \leftarrow \tilde{X}^2\mathrm{A}'$ and the $\tilde{B}^2\mathrm{A}'' \leftarrow \tilde{X}^2\mathrm{A}'$ origin bands in its laser-induced fluorescence (LIF) spectrum. $CaOC_2H_5$ radicals were produced by 1064 nm laser ablation of calcium grains in the presence of ethanol under jet-cooled conditions. Dominant transitions in the vibrationally resolved DF spectra are well reproduced using Franck-Condon factors predicted by complete active space self-consistent (CASSCF) calculations. Differences in transition intensities between the $\tilde{A}^2\mathrm{A}' \rightarrow \tilde{X}^2\mathrm{A}'$ and the $\tilde{B}^2\mathrm{A}'' \rightarrow \tilde{X}^2\mathrm{A}'$ DF spectra are attributed to the pseudo-Jahn-Teller interaction between the $\tilde{A}^2\mathrm{A}'$ and the $\tilde{B}^2\mathrm{A}''$ states. Collision-induced population transfer between these two excited electronic states results in additional peaks in the DF spectra.